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## MARSHALL-PEIERLS SIGN RULE IN FRUSTRATED HEISENBERG CHAINS

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We consider the frustrated antiferromagnetic  $s=1$  Heisenberg quantum spin chain with regard to the Marshall-Peierls sign rule (MPSR). By using exact diagonalization data we investigate the breakdown of the MPSR in dependence on frustration and compare our findings with data for  $s=1/2$ . We calculate a critical value of frustration  $J_2^{crit}$  where the MPSR is violated. The extrapolation of this value to the infinite chain limit holds  $J_2^{crit} \approx 0.016$ , lower than in the case of  $s=1/2$  ( $J_2^{crit} \approx 0.027$ ). This points to a stronger influence of frustration in the case of  $s=1$ . Nevertheless the calculation of the weight of the Ising-states violating the MPSR shows that the MPSR holds approximately even for quite large frustration and may be used for numerical techniques.

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### 1. Introduction

The Marshall-Peierls sign rule (MPSR) determines the sign of the Ising-basis-states building the ground-state wave function of a Heisenberg Hamiltonian [1] and has been proven exactly for bipartite lattices and arbitrary site spins by Lieb, Schultz and Mattis [2]. As pointed out in several papers the knowledge of the sign is of great importance in different numerical methods, e.g. for the construction of variational wave functions [3], in Quantum Monte-Carlo methods (which suffer from the sign problem in frustrated systems [4]) and also in the density matrix renormalization group method, where the application of the MPSR has substantially improved the method in a frustrated spin system [5].

The MPSR has been analyzed so far for systems with  $s=1/2$ . The authors of [6] studied the frustrated chain and found for the ground-state a critical value for the breakdown of the MPSR for the infinite chain limit by using exact diagonalization data. For the  $J_1$ - $J_2$  model on the square lattice the violation of the MPSR was considered as an indication for the breakdown of long range order [7, 8]. In a recent paper [9] we extended these investigations to higher subspaces of  $S^z$ . For linear chains we have shown that for the lowest eigenstates in every subspace of  $S^z$  there is a finite region of frustration where the MPSR holds.

In this paper we want to analyze the frustrated spin chain with  $s=1$ . This spin system has attracted a lot of attention, because of the well known Haldane conjecture [10]. The unfrustrated  $s=1$  spin chain shows a spin gap and exponential decaying correlations whereas the  $s=1/2$  spin chain has no gap and a power-law correlation decay. Since both systems are qualitatively different one might expect also a different influence of frustration on the MPSR.

## 2. The Model and the Marshall-Peierls sign rule

In the following we study the MPSR for the frustrated antiferromagnetic  $s=1$  Heisenberg quantum spin chain:

$$\hat{H} = J_1 \sum_{\langle \text{NN} \rangle} \mathbf{s}_i \mathbf{s}_j + J_2 \sum_{\langle \text{NNN} \rangle} \mathbf{s}_i \mathbf{s}_j, \quad (1)$$

$\langle \text{NN} \rangle$  and  $\langle \text{NNN} \rangle$  denote nearest-neighbor and next-nearest-neighbor bonds on the linear chain. We set  $J_1 = 1$  for the rest of the paper. For this model the MPSR can be exactly proved only for  $J_2 \leq 0$ .

The Marshall-Peierls sign rule can be described as follows: In the unfrustrated limit of  $J_2 = 0$ , the lowest eigenstate of the Hamiltonian (1) in each subspace of fixed eigenvalue  $M$  of the spin operator  $S_{total}^z$  reads

$$\Psi_M = \sum_m c_m^{(M)} |m\rangle, \quad c_m^{(M)} > 0. \quad (2)$$

Here the Ising-states  $|m\rangle$  are defined by

$$|m\rangle \equiv (-1)^{S_A - M_A} |m_1\rangle \otimes |m_2\rangle \otimes \cdots \otimes |m_N\rangle, \quad (3)$$

where  $|m_i\rangle$ ,  $i = 1, \dots, N$ , are the eigenstates of the site spin operator  $S_i^z$  ( $-s_i \leq m_i \leq s_i$ ),  $S_A = \sum_{i \in A} s_i$ ,  $M_{A(B)} = \sum_{i \in A(B)} m_i$ ,  $M = M_A + M_B$ . The lattice consists of two equivalent sublattices  $A$  and  $B$ .  $s_i \equiv s$ ,  $i = 1, \dots, N$ , are the site spins. The summations in Eq.(2) are restricted by the condition  $\sum_{i=1}^N m_i = M$ . The wave function (2) is not only an eigenstate of the unfrustrated Hamiltonian ( $J_2 = 0$ ) and  $S_{total}^z$  but also of the square of the total spin  $\mathbf{S}_{total}^2$  with quantum number  $S = |M|$ . Because  $c_m^{(M)} > 0$  is valid for each  $m$  from the basis set (3) it is impossible to build up other orthonormal states without using negative amplitudes  $c_m^{(M)}$ . Hence the ground-state wave function  $\Psi_M$  is nondegenerated. As it comes out, the MPSR is still fulfilled not only for the ground-state but also for every lowest eigenstate in the subspace  $M$  in the unfrustrated case. We emphasize that for  $J_2 > 0$  no proof for the above statements can be given and that a frustrating  $J_2 > 0$  can destroy the MPSR.

## 3. Results

We have calculated by exact diagonalization the ground-state of the model (1) for  $N=8, \dots, 14$  varying the frustration parameter  $J_2$ . By analyzing the ground-state wave function according to the MPSR we found for every system a critical value of frustration  $J_2^{crit}$ , where the MPSR starts to be violated. We apply the

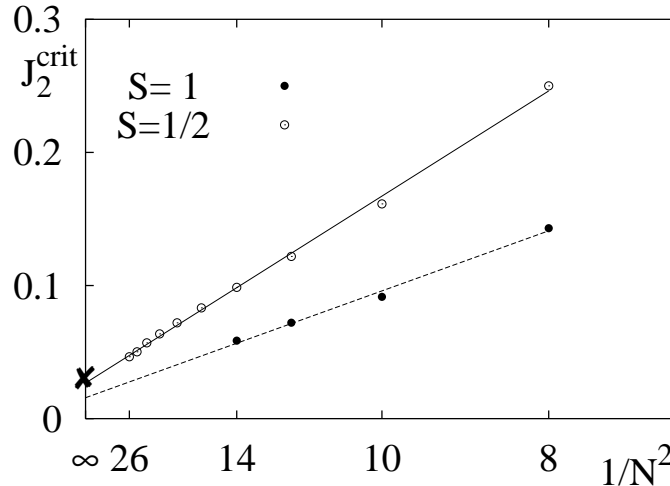


Fig. 1. The critical value of frustration  $J_2^{crit}$ , where the MPSR starts to be violated as a function of the system size  $N$ . The cross denotes the value of Zeng and Parkinson [6].

scaling law proposed by Zeng and Parkinson [6] and extrapolate our data as a function of  $1/N^2$ . We found a value for the infinite chain limit:  $J_2^{crit}(\infty) = 0.016 \pm 0.003$ . In Fig.1 we compare these data with the values for the  $s=1/2$  systems ( $N=8, \dots, 26$ ), where the extrapolation yields  $J_2^{crit}(\infty) = 0.027 \pm 0.003$ . It is also interesting to note that this value is slightly lower than the value of 0.032 found by Zeng and Parkinson [6] using data for  $N=8, \dots, 20$  only.

We argue that in the case of  $s=1$  the chain is more sensitive to frustration and therefore the MPSR is violated for smaller values of  $J_2$ . Nevertheless in numerical methods the MPSR can be used at least approximately for much larger values of frustration. This can be justified by the examination the ground-state wave function according to the Ising-basis-states which violates the MPSR. We call these states non-Marshall-states and denote their weight by  $W_{nM}$ . In Fig.2 we show  $W_{nM}$  as a function of frustration  $J_2$ .

As can be seen in Fig.2, the weight of the non-Marshall-states remains smaller than 1% ( $1E-2$ ) until  $J_2 \approx 0.36$ . This result seems to be more or less size independent because all three lines for the systems with  $N=8, 10$  and  $12$  cross at this point. The points at the bottom line denote the first violation of the MPSR in a given system and coincide with the points given in Fig.1. The examination of  $W_{nM}$  indicates that for quite large frustration the predominant part of the ground-state wave function fulfills the MPSR. Therefore, the MPSR can be used in numerical methods even if it does not hold strictly.

#### 4. Conclusions

We have shown that in the frustrated antiferromagnetic  $s=1$  Heisenberg quantum spin chain the Marshall-Peierls sign rule is violated by frustration. We found by extrapolation to the infinite chain limit a critical value of frustration  $J_2^{crit} \approx 0.016 \pm 0.003$  below which the MPSR still holds exactly. By calculating the weight of the Ising-basis-states of the ground-state wave function which do not

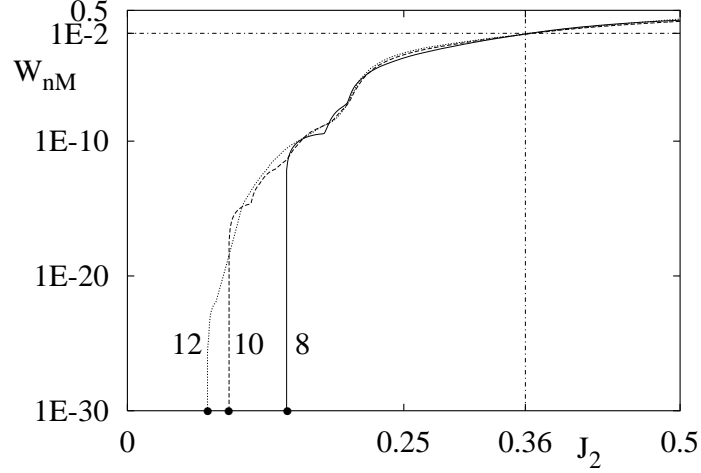


Fig. 2. The weight of non-Marshall-states of the ground-state wave function  $W_{nM}$  as a function of frustration  $J_2$  for systems with  $N=8,10,12$ .

fulfill the MPSR we conclude that the MPSR can be used in numerical methods at least approximately until a large frustration of  $J_2 \approx 0.36$ .

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